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Stable thermodynamic states

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A general class of perturbations of the dynamics for thermodynamic quantum systems is discussed. Without making use of weak asymptotic Abelianess, stability of a state for these perturbations is shown to lead to the ϕ -KMS condition and to the KMS condition in particular cases. Conversely, ϕ -KMS states satisfy the stability property introduced here.

I. INTRODUCTION

The derivation of equilibrium properties for states of thermodynamic systems has already been of interest for some time. It is well known that so-called KMS states may be obtained from stability for perturbation of the dynamics. This has been discussed initially by Haag, Kastler, and Trych-Pohlmeyer, by Kastler and Bratteli, and by Hoekman; for a review cf. Ref. 1, Chap. 5.4.2. However, owing to the assumed rapid decay of the time correlation functions these KMS states can only describe pure thermodynamic phases. A further restriction of the method is that it can be applied only to states of dynamical systems that are weakly asymptotically Abelian; viz. $\int dt \omega([A, \alpha_t B]) = 0$. Here A, B denote elements of the C^* algebra \mathfrak{A} ; $\omega \in E_{\mathfrak{A}}$ is a state over \mathfrak{A} , and $\alpha_t \in \text{aut } \mathfrak{A}$ describes the time evolution.

In this paper we shall discuss a stability property which leads to states that satisfy the ϕ -KMS condition introduced recently.² The main advantage of the stability criterion put forward here is that neither are assumptions made on the decay of the correlation functions nor is the dynamics assumed to act weakly asymptotically Abelian.

Depending on the details of the perturbation for which stability is imposed, the ϕ -KMS states in some cases are KMS states. For an infinite quantum lattice system the ϕ -KMS condition and KMS condition are equivalent.² Consequently, in this instance either our stability condition leads to a KMS state or the system does not admit states that are stable for the particular perturbation. For any finite system or for continuous quantum systems, however, the only states that fulfill the stability criterium are ϕ -KMS states.

For a finite system the presently proposed stability property is stronger than the condition imposed by Lebowitz *et al.*³ For thermodynamic systems our conditions are weaker than those introduced by Kastler⁴ (cf. Ref. 5).

II. A GENERALIZED PERTURBED DYNAMICS

In the Heisenberg picture the equation of motion for the unperturbed evolution reads

$$\frac{d}{dt} \alpha_t(A) = i\alpha_t(\delta(A)), \quad A \in D(\delta) \subset \mathfrak{A}, \quad (2.1)$$

where the derivation δ is the infinitesimal generator of the group of $*$ automorphisms $\{\alpha_t\}$. A perturbed dynamics can be considered as the solution of the differential equation

$$\frac{d}{dt} \tilde{\alpha}_t^h(A) = i\tilde{\alpha}_t^h(\delta(A)) + i\tilde{\alpha}_t^h([h_t, A]), \quad (2.2)$$

cf., e.g., Ref. 6, with $h_t = h^* \in \mathfrak{A}$. One may choose the particular form $h_t = f(t)h$ with $h = h^* \in \mathfrak{A}$ and $f: \mathcal{R} \rightarrow \mathcal{R}$, so that the perturbation becomes localized in time if, e.g., $\text{supp } f$ is compact or $f \in L_1(\mathcal{R})$. The family $\{h_t\}$ can be interpreted as the action of some external agent on the system. Owing to the time dependence of h_t the mappings $\{\tilde{\alpha}_t^h\}$ do not form a group.

A further generalization of the perturbed dynamics is obtained from the following equation of motion:

$$\frac{d}{dt} \tilde{\alpha}_t^h(A) = i\tilde{\alpha}_t^h(\delta(A)) + if_1(t)\tilde{\alpha}_t^h(hA) - if_2(t)\tilde{\alpha}_t^h(Ah). \quad (2.3)$$

The solution to this equation is the family of mappings $\tilde{\alpha}_t^h: \mathfrak{A} \rightarrow \mathfrak{A}$ given by

$$\tilde{\alpha}_t^h(A) = \tilde{\gamma}_t^h(\alpha_t(A)), \quad (2.4a)$$

$$\tilde{\gamma}_t^h(A) = \tilde{u}_t^h(t)A\tilde{u}_t^{h*}(t)^*, \quad (2.4b)$$

$$\tilde{u}_t^h(t) = \sum_{n=0}^{\infty} \left\{ i^n \int_0^t ds_1 \cdots \int_0^{s_{n-1}} ds_n \prod_{k=1}^n [f_j(s_k)\alpha_{s_k}(h)] \right\}, \quad (2.4c)$$

with $f_j \in L_1(\mathcal{R})$ and $h = h^* \in \mathfrak{A}_0$. The unperturbed dynamics α_t is assumed to be strongly continuous on a $\sigma(\mathfrak{A}, N)$ -dense subalgebra $\mathfrak{A}_0 \subset \mathfrak{A}$. Here N denotes the set of locally normal states on \mathfrak{A} (cf. Ref. 7). In general, the mappings $\tilde{\alpha}_t^h$ and $\tilde{\gamma}_t^h$ will not be positivity preserving. The operators $\tilde{u}_t^h(t)$ are easily seen to be unitary. The integrals in (2.4c) exist as Bochner integrals. We now give some useful properties of the generalized perturbed dynamics in the following.

Proposition 2.1: For $A \in \mathfrak{A}$ and $h = h^* \in \mathfrak{A}_0$,

$$\tilde{u}_t^h(t) = \mathbb{1} + i \int_0^t ds f_j(s)\alpha_s(h)\tilde{u}_s^h(s), \quad (2.5a)$$

$$\frac{d}{dt} \tilde{u}_t^h(t) = if_j(t)\alpha_t(h)\tilde{u}_t^h(t); \quad (2.5b)$$

$$\begin{aligned} \tilde{\gamma}_t^h(A) = A + i \int_0^t ds [f_1(s)\tilde{\gamma}_s^h(\alpha_s(h)A) \\ - f_2(s)\tilde{\gamma}_s^h(A\alpha_s(h))], \end{aligned} \quad (2.5c)$$

$$\begin{aligned}\tilde{\alpha}_t^h(A) = & \alpha_t(A) + i \int_0^t ds [f_1(s)\alpha_s(h)\alpha_t(A) \\ & - f_2(s)\alpha_t(A)\alpha_s(h)] + \cdots\end{aligned}\quad (2.5d)$$

The omitted terms in (2.5d) are $O(h^2)$.

Proof: By iteration of (2.5a) we obtain (2.4c). The equivalence of (2.5c) and (2.5b) then follows from the initial condition $\tilde{u}_j^h(0) = 1$. Finally, (2.5c) and (2.5d) are obtained with the use of (2.4b) and (2.4c) along similar lines as in the discussion of the cocycle property (cf., e.g., Ref. 1).

We now turn to the introduction of the notion of stability for perturbations from the unperturbed dynamics α_t as described by (2.5d). Succinctly, one assumes that close to the original state $\omega \in \mathbb{L}^*$ there exists a bounded linear functional $\omega^h \in \mathbb{L}^*$ that is *almost* invariant for the perturbed evolution $\tilde{\alpha}_t^h$. At this point we shall impose some restrictions on the functions f_j .

Definition 2.2: For a pair of functions f_1 and f_2 such that

- (1) $f_j \in L_1(\mathcal{R}) \cap C^1(\mathcal{R})$;
- (2) $\hat{f}_j \in C^\infty(\mathcal{R})$ and invertible on $\text{sp } \alpha$, i.e.,
 $\hat{f}_j(\lambda) \neq 0 \quad \forall \lambda \in \text{sp } \alpha = \{\lambda \in \mathcal{R} \mid \hat{g}(\lambda) \neq 0\}$

$$\forall g: \int dt g(t)\alpha_t(A) = 0$$

$$\forall A \in \mathbb{L}_0\};$$

- (3) $\hat{f}_1(\lambda) = \hat{f}_2(\lambda) \quad \text{iff } \lambda = 0$;

[$\hat{g}(\lambda) = \int dt e^{-i\lambda t} g(t)$ is the Fourier transform] we say that a state ω is (f_1, f_2) -stable if there exists a bounded linear functional $\omega^h \in \mathbb{L}^*$ such that for μ in a neighborhood of the origin

$$\lim_{t \rightarrow \pm \infty} \omega^{\mu h}(\tilde{\gamma}_t^{\mu h} A) = \omega_{\pm}(A); \quad (2.6)$$

$$\omega_+^{\mu h}(A) - \omega_-^{\mu h}(A) = o(\mu); \quad (2.7)$$

and

$$\lim_{\mu \rightarrow 0} \omega^{\mu h}(\alpha_t A) = \omega(\alpha_t A), \quad \text{uniformly in } t \quad (2.8)$$

for all $A \in \mathbb{L}$. With the use of (2.5c) a simple estimate shows that $\omega_+^{\mu h}(A) - \omega_-^{\mu h}(A) = O(\mu)$ so that (2.7) does not seem to be a very severe assumption.

The conditions (2.6) and (2.7) are in fact the same as the ones introduced by Kastler⁴ and Hoekman⁵ because there $\omega^{\mu h}$ is a perturbed state which is invariant for the perturbed dynamics. In Ref. 5 a perturbed dynamics α_t^h is considered that is an Abelian group of transformations. As a consequence, the perturbed state could be explicitly constructed, viz. $\omega^{\mu h}(A) = \mathbb{M}_t \omega(\alpha_t^{\mu h} A)$, where \mathbb{M} is an invariant mean over the additive group of the real numbers and t is a dummy variable.⁸ If, in addition, one has that (\mathbb{L}_0, α_t) is L_1 -asymptotically Abelian, then the convergence (2.8) can be derived.

We shall now proceed with the demonstration that without loss of generality the perturbed state $\omega^{\mu h}$ may be assumed to be *approximately invariant* for the perturbed dynamics.

Lemma 2.3: Let \mathbb{M} be an invariant mean over the addi-

tive group of the real numbers.⁸ Then the time-averaged perturbed state $\mathbb{M}_{t'} \omega^{\mu h}(\alpha_t A) \equiv \mathbb{M} \omega^{\mu h}(A)$, where t' is to be considered as a dummy variable, satisfies

$$\lim_{\mu \rightarrow 0} \mathbb{M} \omega^{\mu h}(\alpha_t A) = \mathbb{M} \omega(\alpha_t A), \quad \text{uniformly in } t \quad (2.9a)$$

and

$$\lim_{\mu \rightarrow 0} [\mathbb{M} \omega^{\mu h}(\tilde{\alpha}_t^h A) - \mathbb{M} \omega^{\mu h}(A)] = 0, \quad \text{uniformly in } t. \quad (2.9b)$$

Proof: Because \mathbb{M} is an invariant mean we have⁸

$$|\mathbb{M}[\omega^{\mu h}(\alpha_t A) - \omega(\alpha_t A)]|$$

$$\leq \sup_{t \in \mathcal{R}} |\omega^{\mu h}(\alpha_t A) - \omega(\alpha_t A)| < \epsilon,$$

for $\mu < \mu_0(\epsilon)$. This establishes the continuity property of the time averaging. Similarly, with the use of (2.5c) we obtain

$$\begin{aligned}|\mathbb{M}[\omega^{\mu h}(\tilde{\alpha}_t^{\mu h} A) - \omega^{\mu h}(A)]| \\ = |\mathbb{M}[\omega^{\mu h}(\tilde{\alpha}_t^{\mu h} A) - \omega^{\mu h}(\alpha_t A)]| \\ \leq \|\omega^{\mu h}\| \|\tilde{\alpha}_t^{\mu h}(A) - \alpha_t(A)\| \\ \leq \|\omega^{\mu h}\| \|\mu\| \|h\| \|A\| (\|f_1\|_1 + \|f_2\|_1),\end{aligned}$$

so that (2.9b) follows from this estimate.

We shall denote the set of $(\check{f}_1, \check{f}_2)$ -stable states by $I_{1,2}$. In order to study the consequences of (f_1, f_2) stability we shall derive a condition which involves only the unperturbed entities ω and α_t and the functions f_1, f_2 . Here $\check{f}(x)$ denotes $f(-x)$.

Proposition 2.4: Let $\omega \in I_{1,2}$ be continuous in the $\sigma(\mathbb{L}, N)$ topology. Then

$$\begin{aligned}\int_{-\infty}^{\infty} dt f_1(t) \omega(A \alpha_t B) \\ = \int_{-\infty}^{\infty} dt f_2(t) \omega(\alpha_t(B) A), \quad \text{for } A, B \in \mathbb{L}.\end{aligned}\quad (2.10)$$

Proof: From Lemma 2.3 it follows that without loss of generality one may assume $\omega^{\mu h}$ to be approximately invariant for $\tilde{\alpha}_t^{\mu h}$, in the sense of (2.9b). For $h = h^* \in \mathbb{L}$, $A \in \mathbb{L}$ we write

$$\int_{T_1}^{T_2} dt \frac{d}{dt} [\omega^{\mu h}(\tilde{\gamma}_t^{\mu h} A)] = \omega^{\mu h}(\tilde{\gamma}_{T_2}^{\mu h} A) - \omega^{\mu h}(\tilde{\gamma}_{T_1}^{\mu h} A).$$

With the use of (2.5c) and (2.6) we find

$$\begin{aligned}\int_{-\infty}^{\infty} dt [\check{f}_1(t) \omega^{\mu h}(\tilde{\alpha}_t^{\mu h}(h \alpha_{-t} A)) \\ - \check{f}_2(t) \omega^{\mu h}(\tilde{\alpha}_t^{\mu h}(\alpha_{-t}(A) h))] \\ = (i/\mu) [\omega_+^{\mu h}(A) - \omega_-^{\mu h}(A)].\end{aligned}$$

The right-hand side vanishes as $\mu \rightarrow 0$ due to (2.7). Because $f_j \in L_1(\mathcal{R})$ the Lebesgue dominated convergence theorem yields for $\mu \rightarrow 0$,

$$\int_{-\infty}^{\infty} dt f_1(t) \omega(h \alpha_t A) = \int_{-\infty}^{\infty} dt f_2(t) \omega(\alpha_t(A) h), \quad (*)$$

for $h = h^* \in \mathbb{L}$ and $A \in \mathbb{L}$. Now consider the GNS representation $(\mathfrak{h}_\omega, \pi_\omega, \Omega_\omega)$ associated with the state ω . Owing to Kaplansky's density theorem $\pi_\omega(h) = \pi_\omega(h)^*$ can be approximated strongly by a net $h_\alpha \in \pi_\omega(\mathbb{L}_0)$ of self-adjoint elements.

With the help of a three- ϵ argument and the polarization method we can now extend (*) to all $h \in \mathbb{H}$.

Throughout this paper we shall adopt the $\sigma(\mathbb{H}, N)$ continuity which we assumed in the preceding proposition.

III. INVARIANCE, SEPARATING CHARACTER, AND THE MODULAR GROUP

From the stability condition (2.11) we now explore the ensuing properties of a state $\omega \in I_{1,2}$. For a state to be stable it should at least be time invariant; i.e., invariant for α_t . To deal with this problem we formulate the following.

Lemma 3.1: (See Ref. 1.) Let F be a bounded function of two variables and $h \in L_1(\mathcal{R})$. If $F(h) = \int ds dt F(s, t) h(s, t)$ vanishes for all h with $\hat{h}(p, q)$ having compact support not containing $q = 0$ and $h(s, t)$ is differentiable with respect to t , with $\partial h(s, t)/\partial t \in L_1(\mathcal{R})$, then

$$F(s, t) = G(s),$$

for some bounded function G . Now we are able to prove the desired invariance.

Proposition 3.2: If $\omega \in I_{1,2}$ then ω is invariant for the unperturbed dynamics α_t .

Proof: Let $A = 1$ and $B = C_g = \int dt g(t) \alpha_t(C)$, then (2.11) yields

$$\omega(C_{h_1} - C_{h_2}) = \omega(C_{h_1 - h_2}) = 0, \quad (3.1)$$

for $C \in \mathbb{H}_0$, $\hat{g} \in D$, and $h_j = f_j * g$. From Lemma 3.1 we now conclude that $\omega(\alpha_t(C))$ is a constant for all $C \in \mathbb{H}_0$. Invoking the continuity of ω yields invariance, viz. $\omega \circ \alpha_t = \omega$.

To proceed further it is now convenient to write the stability condition (2.11) in the GNS representation. Let $(\mathfrak{h}, \pi, \Omega)$ be the GNS triple associated with $\omega \in I_{1,2}$. Since ω is invariant, the group of $*$ automorphisms $\{\alpha_t\}$ can be implemented by a strongly continuous group of unitaries on \mathfrak{h} . To this end we must also assume that the correlation functions $t \rightarrow \omega(A \alpha_t B)$ are continuous. Explicitly, we then have $\pi(\alpha_t(A)) = U_t \pi(A) U_t^*$ and $U_t \Omega = \Omega$. The stability criterion (2.11) can now be written as

$$\int dt f_1(t) (\Omega, A U_t B \Omega) = \int dt f_2(t) (\Omega, B U_t^* A \Omega), \quad (3.2)$$

for $A, B \in \pi(\mathbb{H})$.

The infinitesimal generator of U_t , i.e., the Liouville operator, will be denoted by L , with the spectral representation $L = \int dE_\lambda \lambda$.

Proposition 3.3: If $\omega \in I_{1,2}$ then Ω is separating.

Proof: From (3.2) we have

$$(\Omega, A \hat{f}_1(L) B \Omega) = (\Omega, B \hat{f}_2(L) A \Omega), \quad (3.3)$$

where $\check{f}(\lambda) = f(-\lambda)$. Let $A \Omega = 0$ then

$$(\Omega, A \hat{f}_1(L) B \Omega) = 0,$$

so that

$$(\hat{f}_1(L) A * \Omega, B \Omega) = 0, \quad (3.4)$$

for all $B \in \pi(\mathbb{H})$. Because \hat{f}_1 is invertible on $\text{sp } \alpha = \{\lambda \mid \hat{g}(\lambda) = 0 \forall g: \int g(t) \alpha_t(A) dt = 0 \forall A \in \mathbb{H}_0\} \supset \{\lambda \mid \hat{g}(\lambda) = 0 \forall g: \int g(t) U_t A \Omega dt = 0 \forall A \in \pi(\mathbb{H}_0)\} = \text{sp } L$, f_1 is also invertible on $\text{sp } L$. Since Ω is cyclic it follows now from (3.4) that $A * \Omega = 0$ and therefore $A = 0$ by standard arguments.⁹

As a consequence we have that the state $(\Omega, \cdot \Omega)$ is a Tomita state on $\pi(\mathbb{H})$ with the modular automorphism $\sigma_t(\cdot) = \Delta^{it} \cdot \Delta^{-it}$, where Δ is the modular operator.

The preceding results already show great similarity of the (f_1, f_2) -stable states with thermodynamic equilibrium states. We shall make this connection more explicit in the following.

Theorem 3.4: If $\omega \in I_{1,2}$ with $f_{1,2}$ such that $\phi(\lambda) = \hat{f}_1(\lambda)/\hat{f}_2(\lambda)$ satisfies

(i) $\phi(\lambda) \check{\phi}(\lambda) = 1$, with $\check{\phi}(\lambda) = \phi(-\lambda)$;

(ii) $\phi(\lambda) > 0$ for $\lambda \in \text{sp } L$;

then $\omega \in K_\phi$, i.e., ω is a ϕ -KMS state.

Whenever (i) and (ii) are not fulfilled $I_{1,2} = \emptyset$. Conversely, if $\omega \in K_\phi$ then $\omega \in I_{1,2}$ for some nonunique $f_{1,2}$ such that $\hat{f}_1/\hat{f}_2 = \phi$.

Proof: Suppose $\omega \in I_{1,2}$, then from (3.3) it follows that

$$(A * \Omega, \hat{f}_1(L) B \Omega) = (B * \Omega, \hat{f}_2(L) A \Omega).$$

Now choose $A = A_g$ with $\hat{g} = \check{f}_1$ then

$$\begin{aligned} & (\check{f}_1(L) A * \Omega, \hat{f}_1(L) B \Omega) \\ &= (B * \Omega, \hat{f}_2(L) \check{f}_1(L) A \Omega) \\ &= (\check{f}_1(L) B * \Omega, [\hat{f}_2(L)] / [\hat{f}_1(L)] \check{f}_1(L) A \Omega). \end{aligned}$$

Furthermore, we may let $B = A *$ and since we assumed $\phi = \hat{f}_1/\hat{f}_2 > 0$ on $\text{sp } L$ we have

$$\|\check{f}_1(L) A * \Omega\| = \|\check{\phi}(L)^{1/2} \check{f}_1(L) A \Omega\|. \quad (3.5)$$

Since $\hat{f}_1(L)$ is invertible we can use the same reasoning as in Ref. 5 to conclude from (3.5) that the modular operator Δ can be written

$$\Delta^2 = \check{\phi}(L) = \left[\frac{\hat{f}_1(L)}{\hat{f}_2(L)} \right]^\sim = \frac{\hat{f}_2(L)}{\hat{f}_1(L)}. \quad (3.6)$$

It was shown in Ref. 2 that (3.6) is equivalent with $\omega \in K_\phi$.

The proof of the converse is quite easy. If $\omega \in K_\phi$ then

$$\int dt f_\phi(t) \omega(A \alpha_t B) = \int dt f(t) \omega(\alpha_t(B) A), \quad (3.7)$$

for all $A, B \in \mathbb{H}$, $\hat{f} \in D$, and $\hat{f}_\phi = \phi \hat{f}$, with $\phi \in C^\infty(\mathcal{R})$. Now choose $\hat{F} \neq 0$ on $\text{sp } L$ and a sequence $(\hat{g}_n)_{n=1}^\infty$ in D , such that $\hat{g}_n \rightarrow \hat{F}$ and $\phi \hat{g}_n \rightarrow \phi \hat{F}$ in S . As ϕ may have an essential singularity at infinity, owing to a theorem of Weierstrass, we can write $\phi = \exp(g)$. Here g is odd and finite in the finite complex plane. Now choose a function h with a Laurent expansion such that $\psi = \exp(h) \in S$ and $\phi \psi \in S$. Then we have for any $\hat{G} \in S$ that $\hat{F} = \psi \hat{G} \in S$ and $\phi \hat{F} = (\phi \psi) \hat{G} \in S$. Then it follows that ω satisfies (2.11), with $f_1 = F_\phi$ and $f_2 = F$, where $F, F_\phi \in L_1(\mathcal{R}) \cap C^1(\mathcal{R})$. Obviously we have $\hat{f}_1/\hat{f}_2 = \phi$; and since $\check{\phi}(L) = \Delta^2$, (3.7) can only be satisfied if on $\text{sp } L$ $\phi > 0$ and $\phi \check{\phi} = 1$ (Ref. 2, Lemma 4).

We conclude with a further remark which can now be made regarding the set $I_{1,2}$.

Remark 3.5: From (3.6) it follows that the modular operator Δ commutes with the Liouville operator L . Then one may follow the line of reasoning given in Ref. 10 to establish that $I_{1,2}$ is a lattice in its own order. In general $I_{1,2}$ will not be closed and hence *a fortiori* not compact. If one assumes in addition the compactness of $I_{1,2}$ in the w^* topology, then it follows that $I_{1,2}$ is a Choquet simplex.

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